FIG.1

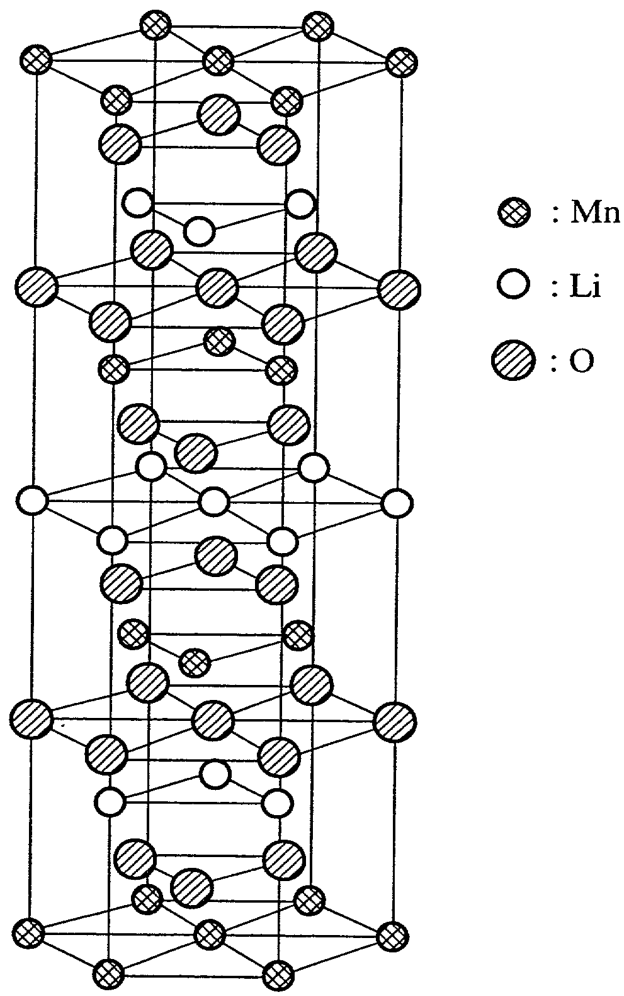

FIG.2

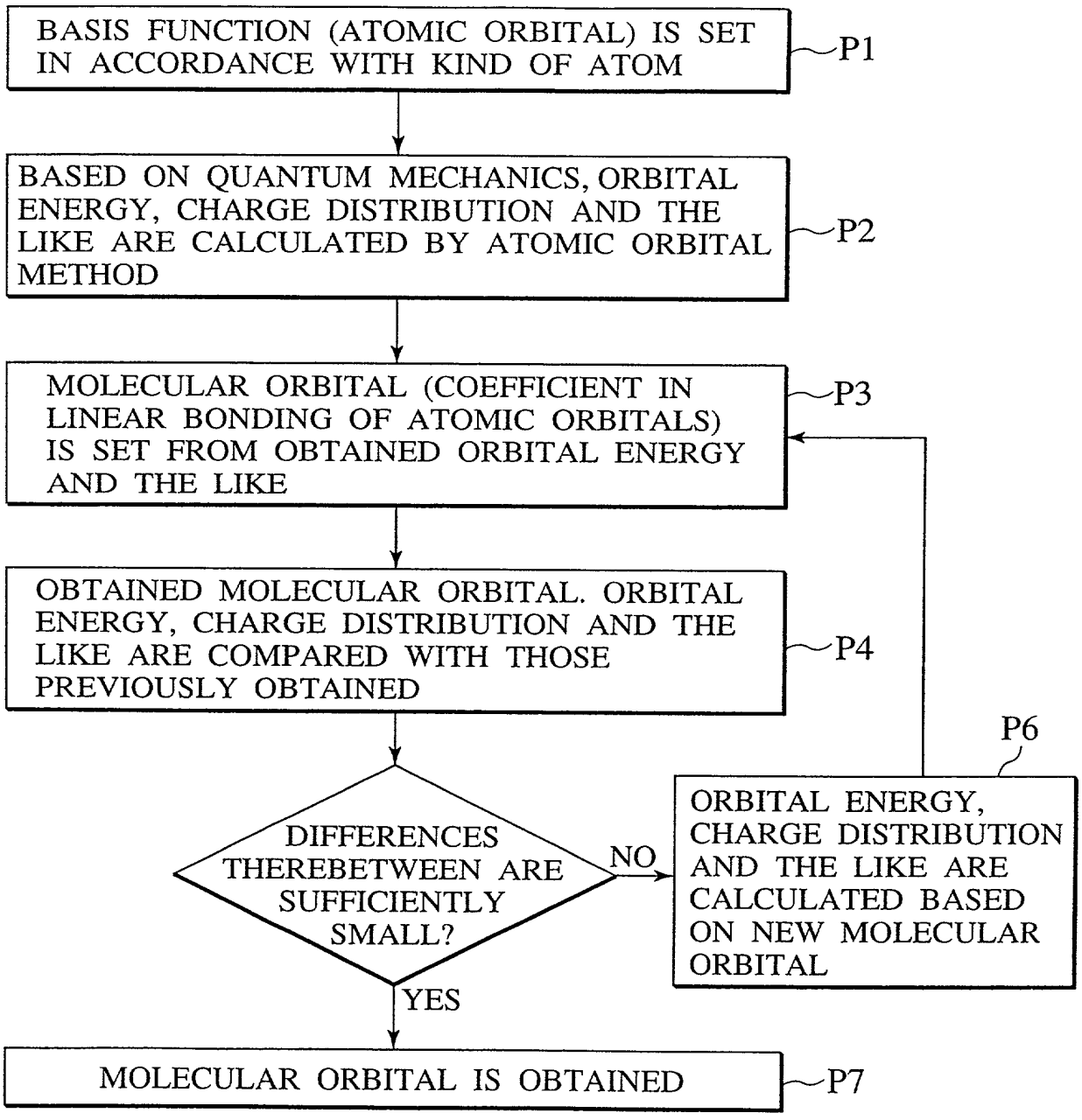
BASIS FUNCTION (ATOMIC ORBITAL) IS SET IN ACCORDANCE WITH KIND OF ATOM
P1
BASED ON QUANTUM MECHANICS, ORBITAL ENERGY, CHARGE DISTRIBUTION AND THE LIKE ARE CALCULATED BY ATOMIC ORBITAL METHOD
P2
MOLECULAR ORBITAL (COEFFICIENT IN LINEAR BONDING OF ATOMIC ORBITALS) IS SET FROM OBTAINED ORBITAL ENERGY AND THE LIKE
P3
OBTAINED MOLECULAR ORBITAL. ORBITAL ENERGY, CHARGE DISTRIBUTION AND THE LIKE ARE COMPARED WITH THOSE PREVIOUSLY OBTAINED
P4
DIFFERENCES THEREBETWEEN ARE SUFFICIENTLY SMALL?
NO
YES
P6
ORBITAL ENERGY, CHARGE DISTRIBUTION AND THE LIKE ARE CALCULATED BASED ON NEW MOLECULAR ORBITAL
MOLECULAR ORBITAL IS OBTAINED
P7

FIG.3

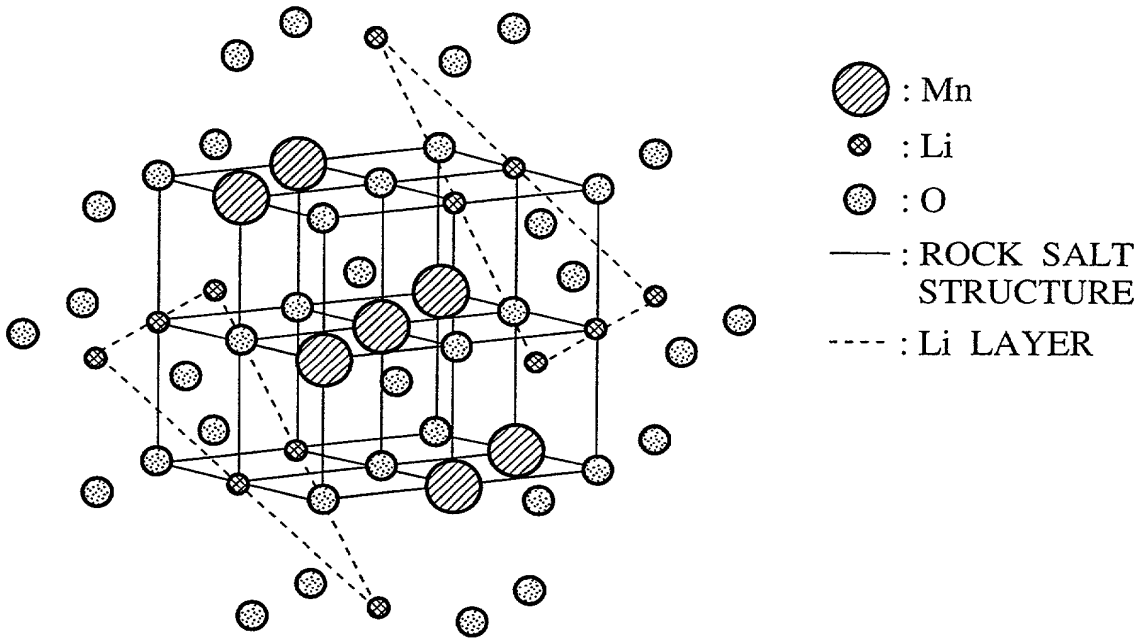
: Mn
: Li
: O
: ROCK SALT STRUCTURE
: Li LAYER

FIG.4

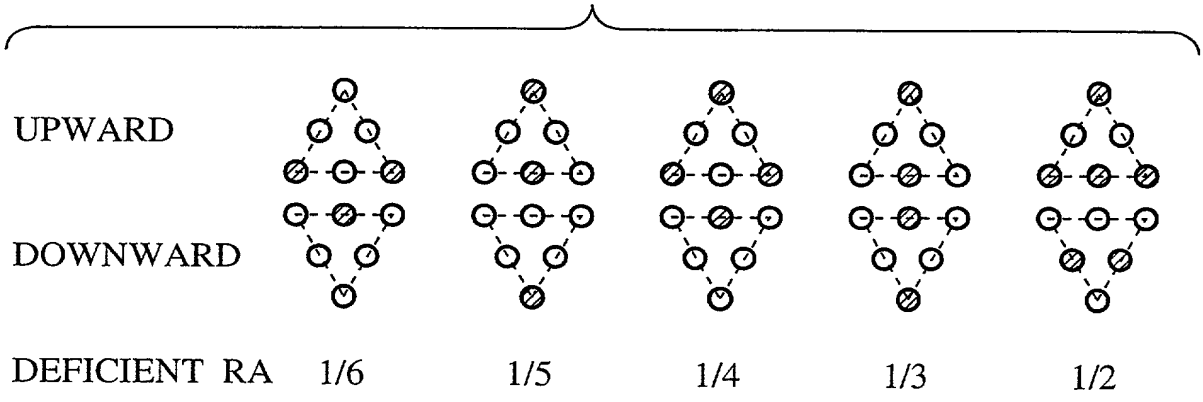
UPWARD
DOWNWARD
DEFICIENT RA
1/6
1/5
1/4
1/3
1/2
: Li
: Li-DEFICIENCY
: Li LAYER IN FIG.3

FIG.5

	Mole ratio of each element in positive electrode material		Composition of positive electrode	Theoretical capacity (mAh/g)	BOP (−)	Relative BOP (−)
	Li	Mn				
Example 1	0.75 (x=1/4)	1.00	$Li_{0.75}MnO_{2-\delta}$	222	0.23	1.28
Example 2	0.7 (x=3/10)	1.00	$Li_{0.7}MnO_{2-\delta}$	207	0.23	1.28
Example 3	0.67 (x=1/3)	1.00	$Li_{0.67}MnO_{2-\delta}$	197	0.23	1.28
Example 4	0.6 (x=2/5)	1.00	$Li_{0.5}MnO_{2-\delta}$	178	0.24	1.33
Comparative example 1	0.5 (x=1/2)	1.00	$Li_{0.5}MnO_{2-\delta}$	148	0.24	1.33
Comparative example 2	1.00	1.00	$LiMnO_{2-\delta}$	296	0.18	1.00
Comparative example 3	0.83 (x=1/6)	1.00	$Li_{0.83}MnO_{2-\delta}$	247	0.21	1.17
Comparative example 4	0.8 (x=1/5)	1.00	$Li_{0.8}MnO_{2-\delta}$	237	0.21	1.17

FIG.6

	Mole ratio of each element in positive electrode material				Composition of positive electrode	BOP (−)	Relative BOP (−)
	Li	Mn	Fe	Ni			
Example 5	0.75	0.67	0.33	0	$Li_{0.76}Mn_{0.67}Fe_{0.33}O_{2-\delta}$	0.23	1.28
Example 6	0.75	0.67	0	0.33	$Li_{0.75}Mn_{0.67}Ni_{0.33}O_{2-\delta}$	0.24	1.33
Example 7	0.75	0.75	0.25	0	$Li_{0.75}Mn_{0.75}Fe_{0.25}O_{2-\delta}$	0.24	1.33
Example 8	0.75	0.75	0	0.25	$Li_{0.75}Mn_{0.75}Ni_{0.25}O_{2-\delta}$	0.24	1.33
Example 9	0.67	0.67	0.33	0	$Li_{0.67}Mn_{0.67}Fe_{0.33}O_{2-\delta}$	0.24	1.33
Example 10	0.67	0.67	0	0.33	$Li_{0.67}Mn_{0.67}Ni_{0.33}O_{2-\delta}$	0.24	1.33

FIG.7

	Composition of positive electrode	Theoretical capacity / (mAh/g)	BOP (−)	Relative BOP (−)
Example 11	$Li_{0.75}Mn_{0.67}Cr_{0.33}O_{2-\delta}$ ($\delta \leqq 0.2$)	222	0.238	1.32
Example 12	$Li_{0.75}Mn_{0.67}Co_{0.33}O_{2-\delta}$ ($\delta \leqq 0.2$)	222	0.235	1.31
Example 13	$Li_{0.75}Mn_{0.33}(Cr_{0.5}Co_{0.5})_{0.67}O_{2-\delta}$ ($\delta \leqq 0.2$)	222	0.239	1.33
Example 14	$Li_{0.75}Mn_{0.5}(Cr_{0.8}Al_{0.2})_{0.5}O_{2-\delta}$ ($\delta \leqq 0.2$)	222	0.240	1.33
Example 15	$Li_{0.75}Mn_{0.5}(Cr_{0.4}Co_{0.4}Al_{0.2})_{0.5}O_{2-\delta}$ ($\delta \leqq 0.2$)	222	0.242	1.34
Comparative example 5	$Li_{0.8}Mn_{0.67}Cro_{0.33}O_{2-\delta}$ ($\delta \leqq 0.2$)	237	0.213	1.18
Comparative example 6	$Li_{0.67}Mn_{0.37}Co_{0.33}O_{2-\delta}$ ($\delta \leqq 0.2$)	197	0.236	1.31

FIG.8

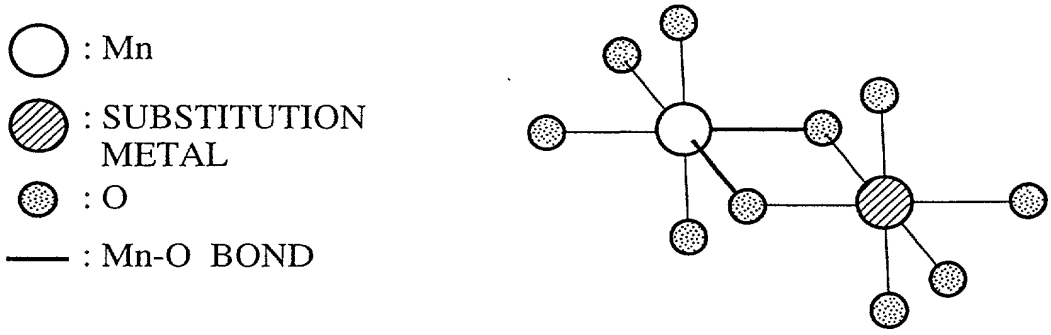
: Mn
: SUBSTITUTION METAL
: O
: Mn-O BOND

FIG.9

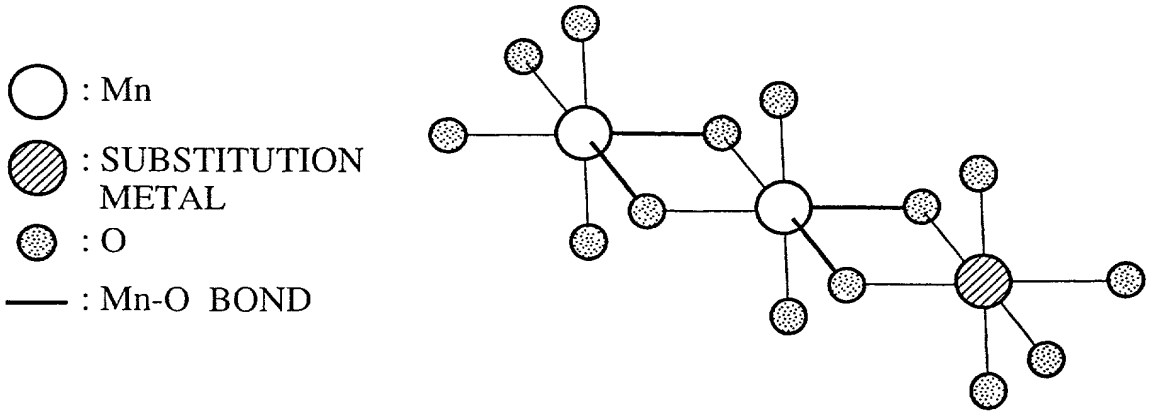
: Mn
: SUBSTITUTION METAL
: O
: Mn-O BOND

FIG.10

	Mole ratio of each element in positive electrode material		Composition of positive electrode	Relative BOP (−)
	Mn	Substitusion metal		
Example 16	0.5 (y=1/2)	Cr, 0.5	$Li_{1-x}Mn_{0.5}Cr_{0.5}O_{2-\delta}$	2.61
Example 17	0.5(y=1/2)	Fe, 0.5	$Li_{1-x}Mn_{0.5}Fe_{0.5}O_{2-\delta}$	1.57
Example 18	0.5 (y=1/2)	Ni, 0.5	$Li_{1-x}Mn_{0.5}Ni_{0.5}O_{2-\delta}$	1.11
Comparative example 7	1.0 (y=1)	0	$Li_{1-x}MnO_{2-\delta}$	1.00
Comparative example 8	0.5 (y=1/2)	Co, 0.5	$Li_{1-x}Mn_{0.5}Co_{0.5}O_{2-\delta}$	0.71
Example 19	0.67 (y=1/3)	Cr, 0.33	$Li_{1-x}Mn_{0.67}Cr_{0.33}O_{2-\delta}$	2.61
Example 20	0.67 (y=1/3)	Fe, 0.33	$Li_{1-x}Mn_{0.67}Fe_{0.33}O_{2-\delta}$	1.97
Example 21	0.67 (y=1/3)	Ni, 0.33	$Li_{1-x}Mn_{0.67}Ni_{0.33}O_{2-\delta}$	2.12
Comparative example 9	1.0 (y=1)	0	$Li_{1-x}MnO_{2-\delta}$	1.00
Comparative example 10	0.67 (y=1/3)	Co, 0.33	$Li_{1-x}Mn_{0.67}Co_{0.33}O_{2-\delta}$	0.96

FIG.11

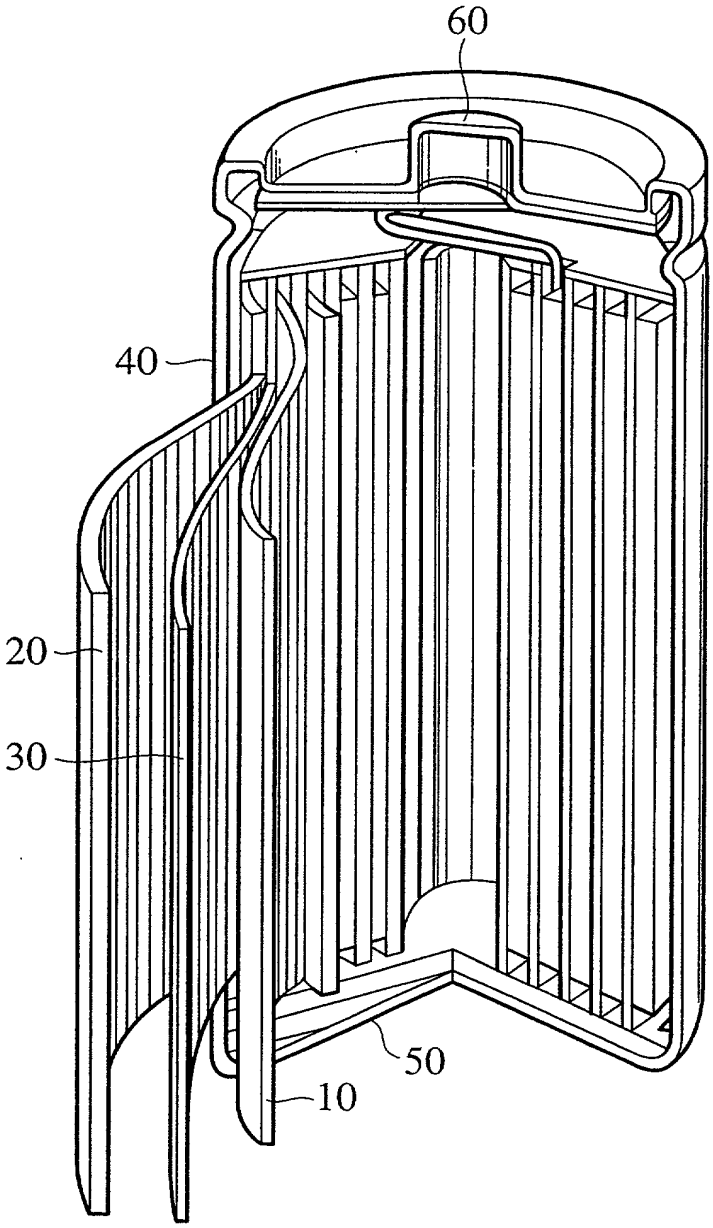

FIG.12A

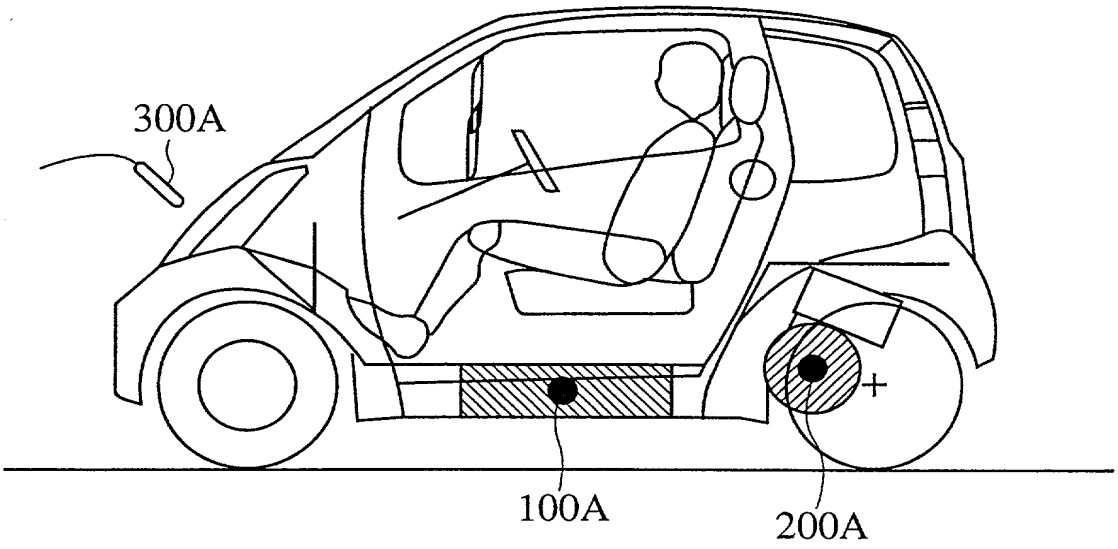

FIG.12B